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FOR BASIC SCIENCES**

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DEPARTMENTAL SEMINAR

Condensed Matter and Materials Physics

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SPEAKER

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TITLE OF THE TALK

**STUDY ON OPTICAL AND ELECTRICAL TRANSPORT PROPERTIES OF TWISTED
BILAYER TRANSITION METAL DICHALCOGENIDES**

ABSTRACT

Van der Waals (vdW) heterostructures, where dissimilar atomically thin vdW crystals are vertically assembled, have initiated a new paradigm to create flexible multifunctional devices. Despite the weak nature of vdW interactions, unusually strong interlayer coupling and hybridization in these heterostructures lead to novel physical phenomena ranging from interfacial stress fields to modification of electronic band structure. In twisted van der Waals heterostructures (vdWHs), the angular mismatch between two similar lattices generates a large-scale interference pattern, known as the moiré pattern, which strongly impacts the electronic band structure of the superlattice. The moiré patterns in vdWHs create a periodic potential for electrons and excitons to yield many interesting phenomena such as Hofstadter butterfly spectrum, moiré excitons, tunable Mott insulator phases, unconventional superconductivity. In this talk I will explain, the effects of moiré patterns on twisted TMDC bilayers by using Raman and PL measurements and try to probe the modified electronic properties in moiré superlattice through transport measurements.

The relative rotation between the adjacent layers or the twist angle between them plays a crucial role in changing the electronic band structure of the superlattice. The first part of the thesis attempts to create such twisted TMDC bilayers with highly accurate twist angle. The assembly of multi-layers of precisely twisted two-dimensional layered materials requires knowledge of the atomic structure at the edge of the flake. At the beginning of this thesis, we demonstrate a simple and elegant transfer protocol using only optical microscope as an edge identifier tool. In this method, controlled transfer of twisted homobilayer and heterobilayer transition metal dichalcogenides is performed with close to 100% yield. The fabricated twisted van der Waals heterostructures have been characterized by SHG, Raman spectroscopy, and photoluminescence spectroscopy, confirming the desired twist angle within 0.5° accuracy. The presented method is reliable, quick, and prevents the use of invasive tools, which is desirable for reproducible device functionalities.

Subsequently, we have studied the phonon renormalization in twisted bilayers of MoS₂, which adds insight to the moiré physics. The interlayer coupling in these heterostructures is sensitive to twist angles (θ) and key to controllably tuning several exotic properties. We demonstrate a systematic evolution of the interlayer coupling strength with twist angle in bilayer MoS₂ using a combination of Raman spectroscopy and simulations. In the absence of doping, we show a monotonic increment of the separation between the A_{1g} and E_{2g} mode frequencies as θ decreases from 10° to 1°, which saturates to that for a bilayer at small twist angles. Furthermore, we use doping-dependent Raman spectroscopy to reveal θ -dependent softening and broadening of the A_{1g} mode, whereas the E_{2g} mode remains unaffected. Using first principles-based simulations, we demonstrate large (weak) electron-phonon coupling for the A_{1g} (E_{2g}) mode, explaining the observed trends. Our study provides a non-destructive way to characterize the twist angle and the interlayer coupling and establishes the manipulation of phonons in twisted bilayer MoS₂ (twistronics).

Besides the closely aligned moiré lattice, bilayers at intermediate misorientation (twist angles θ ; 15°) also offer a unique opportunity to tune optically excited states. To explore the light-matter interaction at an intermediate angle, we have then explored many-body excitonic complexes in monolayer (ML), natural bilayer (BL), and twisted bilayer (tBL) WSe₂ with Raman and Photoluminescence spectroscopy. We observed signatures of neutral biexciton (XX) in tBL, for the first time, but not in non-encapsulated ML and BL, demonstrating the unique effects of disorder screening in twisted bilayers. The XX, as well as charged biexciton (XX⁻), are robust to thermal dissociation and are controllable by electrostatic doping. Vanishing of momentum-indirect interlayer excitons with increasing electron doping is demonstrated in tBL, resulting from near-alignment of Q⁻-K and K-K valleys. Intermediate misorientation samples offer a high degree of control of excitonic complexes while offering possibilities for studying exciton-phonon coupling, band-alignment, and screening.

Finally, we investigated electrical transport in Graphene/twisted WSe₂ heterostructure, using graphene as a sensing layer to probe the electronic effects of the underlying twisted TMDC structure on monolayer graphene. Unlike graphene, metal-TMDC contacts are highly resistive. We used metals of different work function to reduce the Schottky barrier across the metal-semiconductor junction.

However, getting a low resistance ohmic contact between the metal-TMDC junction to probe electronic states in the twisted bilayers directly has been difficult. We bypassed this issue by using graphene as a sensing layer in monolayer graphene/tWSe₂-based heterostructures. Our measurements show likely signatures of out-of-plane ferroelectricity in the twisted bilayers, which manifest in hysteretic transfer characteristics. We also find a huge nonlocal signal in graphene at a zero magnetic field that cannot be explained via classical contribution. Both the nonlocal and local resistance can be controlled through the electric field. We further explore the magneto transport properties of the system and find that the magnetoresistance of the sample increases with an in-plane magnetic field.

HOST FACULTY

Dr. Atindra Nath Pal
